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An Algorithm for Isotonic Regression in the Plane

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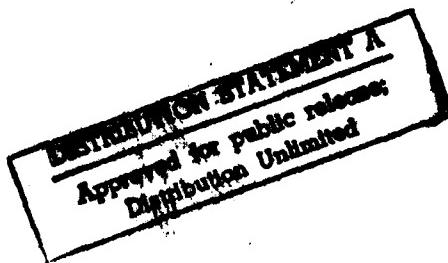
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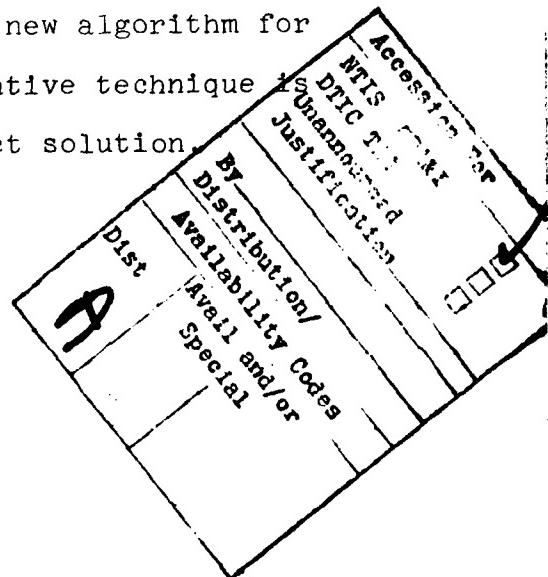
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(University of Missouri, Columbia and University of Iowa)

ABSTRACT

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Key Words and Phrases: Isotone regression, minimal lower sets
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1. INTRODUCTION.   Algorithms for calculating the least

squares isotonic regression function have received a great deal

of attention in the literature and six such algorithms are dis-

cussed in Section 2.3 of Barlow, Bartholomew, Bremner and

Brunk (1972).   In situations where there is one independent

variable all of the algorithms work very efficiently.   Perhaps

the most widely used algorithm is the "pool adjacent violators

algorithm" which is applicable only in the case of a simple

linear ordering or an amalgamation of simple orderings.   In

many isotonic regression problems we have more than one inde-

pendent variable present and are concerned with partial order-

ings.   An important example involves the prediction of success

in college.   Usually, this prediction is based upon several

independent variables such as rank in high school graduating

class and score on a standardized examination such as the ACT

composite and is measured in terms of a predicted grade point

average or predicted probability of obtaining a particular GPA

or better.   The predicted value is usually obtained by regres-

sion methods and is assumed to be nondecreasing in each inde-

pendent variable.   The isotonic regression function has been

found to compare very favorably with other techniques with

respect to predictive accuracy (cf. Perrin and Whitney (1976)

and Kolen and Whitney (1978)).

Some of the algorithms described in Barlow et al. are

applicable to the case of computing the doubly nondecreasing

least squares regression function but the number of computations required can become prohibitive. For example, consider the minimum lower sets algorithm described in Section 2.3 of Barlow et al. Suppose one of our two independent variables has a possible values and the other has b possible values. By counting paths from the upper left hand corner to the lower right hand corner of our a x b grid, it follows that the number of lower sets is equal to $\binom{a+b}{a}$. If a = b this number is approximately $(a\pi)^{-1/2} \cdot 4^a$ by Stirling's formula. Thus if a = b = 20, and if consideration of each lower set were to require one microsecond of computer time, then finding the first level set would require 2312 minutes or 38.5 hours of CPU time. (One microsecond seems conservative in light of the fact that computation of the average value over that set would take at least two multiplications, two additions and a division and the comparison would require a subtraction. The present standard for making such predictions is four arithmetic operations per microsecond.) Moreover, if the first level set is small (as it would be with good data) the second cycle is nearly as difficult as the first, etc.

Since the doubly nondecreasing regression function is so difficult to compute, researchers have proposed using ad hoc estimators based upon one dimensional smoothings. (The number of computations required for one dimensional smoothings is essentially linear in the number of entries.) Makowski (1974) studied consistency properties of estimators obtained by

successive one dimensional smoothings. Kolen, Smith and Whitney
(1977), Perrin and Whitney (1976), and Kolen and Whitney (1978)
proposed two different techniques for producing estimates which
are nondecreasing in each variable. One of their techniques
was to first do one dimensional row smoothings. After all rows
had been adjusted, reversals in the columns were adjusted by
the same method. They then returned to the original table and
did one dimensional column smoothing followed by row smoothings.
Neither smoothing necessarily produces a doubly nondecreasing
table so   they averaged the two results. (The average is
not necessarily doubly nondecreasing but was for their data.)
This method was applied to the problem of estimating the prob-
ability of obtaining a "B or better" GPA for entering college
students. The data is presented in Table 1. The two entries
are the total cell frequencies and the observed relative fre-
quencies. We note that there are a number of "reversals,"
even with a relatively large sample size. The smoothed esti-
mates, by their method, are presented in Table 2 and the iso-
tonic regression function with weights equal to frequencies
in Table 3. Note that not only the estimates but also the level
sets are different. These level sets are very useful for making
inferences about equivalent scores within the table.

Several of the algorithms discussed in Section 2.3 of
Barlow et al. are basically methods of finding linear orders
which are consistent with a partial order. We have not been
able to write a program which implements any of these methods

TABLE 1

The probability of making a "B or better" GPA
(top number = total cell frequency; bottom number = relative frequency)

ACT Composite	High School Grade Point Average				
	0 to 1.55	1.56 to 2.25	2.26 to 2.95	2.96 to 3.65	3.66 to 4.00
28[+]	0 .0000	7 .2857	10 .2000	47 .5745	44 .8864
23-27	7 .0000	56 .1250	88 .1818	180 .2833	84 .5238
18-22	23 .0435	166 .0301	152 .0724	149 .1946	33 .1212
13-17	27 .0000	149 .0470	96 .0313	61 .0492	4 .5000
0-12	10 .0000	57 .0000	33 .0606	7 .0000	0 .0000

TABLE 2

The probability of making a "B or better" GPA
Kolen and Whitney Method

.0314	.2353	.2353	.5745	.8864
.0314	.1250	.1818	.2833	.5238
.0314	.0375	.0724	.1867	.1934
.0000	.0375	.0402	.0493	.1784
.0000	.0000	.0383	.0421	.0425

TABLE 3

The probability of making a "B or better" GPA
Least squares isotonic regression (weights = cell frequencies)

.0333	.2353	.2353	.5745	.8864
.0333	.1250	.1818	.2833	.5238
.0333	.0377	.0724	.1881	.1881
.0000	.0377	.0377	.0492	.1881
.0000	.0000	.0377	.0377	.0377

for a doubly nondecreasing regression function in a reasonable amount of time.

In this paper we present an algorithm for calculating the least squares isotonic regression function which is increasing in each of two variables. This algorithm uses successive one dimensional smoothings and is very efficient and easy to program. To illustrate, we applied the algorithm to a 20 by 20 table of random numbers. The isotonic regression was obtained, correct to four significant digits, after 400 iterations, required 39 seconds of CPU time at a cost of one dollar and thirty-five cents. This algorithm is described in Section 3. In Section 2 we summarize some well known properties of isotonic regression which will be used in the proof that the algorithm yields the desired result.

2. SOME PRELIMINARIES. We let $\Omega = \{(i,j); i = 1,2,\cdots,a; j = 1,2,\cdots,b\}$ and define the partial order $\ll$ on Ω by $(i,j) \ll (k,\ell)$ if and only if $i-k \leq 0$ and $j-\ell \leq 0$. We denote an arbitrary real function whose domain is Ω as a matrix, i.e.,

$$G = (g_{ij}) = (g((i,j))), \quad i = 1,2,\cdots,a; j = 1,2,\cdots,b.$$

(Note that this is not the usual matrix notation where g_{ij} refers to the entry in the $i^{\underline{th}}$ row and $j^{\underline{th}}$ column.)

We say that a function $F : \Omega \to R$ is isotonic or order preserving if $(i,j) \ll (k,\ell)$ implies $f_{ij} \leq f_{k\ell}$. This is equivalent to requiring that F be nondecreasing along both rows and columns. The least squares isotonic regression problem is to

$$\text{Minimize} \quad \Sigma_{i,j}(g_{ij} - f_{ij})^2 w_{ij}$$

for F belonging to the class, K, of isotonic functions where $w_{ij} > 0$ and G are given.

Since the class of isotonic functions forms a closed convex cone, it is well known (for example, see Theorem 7.8 in Barlow et al.) that the solution to the isotonic regression problem, say G^*, is characterized by the properties, $G^* \in K$,

$$(2.1) \qquad \Sigma_{i,j}(g_{ij} - g_{ij}^*)g_{ij}^* w_{ij} = 0, \quad \text{and}$$

$$(2.2) \qquad \Sigma_{i,j}(g_{ij} - g_{ij}^*)h_{ij} w_{ij} \leq 0,$$

for all functions $H \in K$.

3. THE ALGORITHM. The algorithm which we propose requires only the ability to solve the isotonic regression problem with the usual nondecreasing order (in one dimension) along rows and columns. Our algorithm is given as follows:

1. Let $\hat{G}^{(1)} = (\hat{g}_{ij}^{(1)})$ denote the isotonic regression solution of $G = (g_{ij})$ over rows, i.e., $\hat{G}^{(1)}$ minimizes $\sum_{i=1}^{a} (g_{ij}-f_{ij})^2 w_{ij}$ subject to $f_{1j} \le f_{2j} \le \cdots \le f_{aj}$ for $j = 1, \cdots, b$. We call $R^{(1)} = (r_{ij}^{(1)}) = (\hat{g}_{ij}^{(1)} - g_{ij})$ the first set of "row increments."

2. Let $\tilde{G}^{(1)} = (\tilde{g}_{ij}^{(1)})$ denote the isotonic regression solution over columns from the initial values $G + R^{(1)}$, i.e., $\tilde{G}^{(1)}$ minimizes $\sum\limits_{j=1}^{b} (g_{ij} + r_{ij}^{(1)} - f_{ij})^2 w_{ij}$ subject to $f_{i1} \leq f_{i2} \leq \cdots \leq f_{ib}$ for $i = 1, \cdots, a$. We call $C^{(1)} = \tilde{G}^{(1)} - (G + R^{(1)})$ the first set of "column increments." Note that $\tilde{G}^{(1)} = G + R^{(1)} + C^{(1)}$.

3. Etc. At the beginning of the nth cycle, we obtain $\hat{G}^{(n)}$ by isotonizing $G + C^{(n-1)}$ over rows. The nth set of row increments is defined by $R^{(n)} = \hat{G}^{(n)} - (G + C^{(n-1)})$ so that $\hat{G}^{(n)} = G + C^{(n-1)} + R^{(n)}$. We then obtain $\tilde{G}^{(n)}$ by isotonizing $G + R^{(n)}$ over columns. The nth set of column increments is given by $C^{(n)} = \tilde{G}^{(n)} - (G + R^{(n)})$, or equivalently $\tilde{G}^{(n)} = G + R^{(n)} + C^{(n)}$.

The utility of the algorithm lies in the following theorem.

<u>Theorem 3.1.</u> Both $\hat{G}^{(n)}$ and $\tilde{G}^{(n)}$ converge to the true solution G^* as $n \to \infty$.

<u>Proof.</u> If we denote the inner product norm as

$$\|F\| = (F,F)^{\frac{1}{2}} = \left(\sum_{i=1}^{a} \sum_{j=1}^{b} f_{ij}^2 w_{ij} \right)^{\frac{1}{2}},$$

we first show

$$(3.1) \qquad \|\hat{G}^{(n)}\|^2 \geq \|\tilde{G}^{(n)}\|^2 \geq \|\hat{G}^{(n+1)}\|^2 \quad \text{for all} \quad n.$$

To establish some additional notation, we denote the "row cone" by

$$K_r = \{F; \ f_{1j} \leq f_{2j} \leq \cdots \leq f_{aj} \quad \text{for} \quad j = 1, \cdots, b\},$$

and the "column cone" by

$$K_c = \{F; \ f_{i1} \leq f_{i2} \leq \cdots \leq f_{ib} \quad \text{for} \quad i = 1, \cdots, a\}.$$

The respective dual cones, as discussed in Barlow and Brunk (1972), are

$$K_r^{*W} = \{H; \ \sum_{i=1}^{a} h_{ij} f_{ij} w_{ij} \leq 0 \quad \text{for} \quad j = 1, \cdots, b; \text{ for every } F \in K_r\}$$

and

$$K_c^{*W} = \{H; \ \sum_{j=1}^{b} h_{ij} f_{ij} w_{ij} \leq 0 \quad \text{for} \quad i = 1, \cdots, a; \text{ for every } F \in K_c\}.$$

Since $-R^{(n+1)}$ is the projection of $G + C^{(n)}$ onto K_r^{*W}, the work of Barlow and Brunk guarantees that

$$-R^{(n+1)} \quad \text{minimizes} \quad \|G + C^{(n)} - F\|^2 \quad \text{for} \quad F \in K_r^{*W}.$$

Similarly,

$$-C^{(n)} \quad \text{minimizes} \quad \|G + R^{(n)} - F\|^2 \quad \text{for} \quad F \in K_c^{*W}.$$

Therefore, since $-R^{(n)} \in K_r^{*w}$ and $-C^{(n-1)} \in K_c^{*w}$,

$$\|G + R^{(n)} - (-C^{(n-1)})\|^2 \geq \|G + R^{(n)} - (-C^{(n)})\|^2 \geq \|G + C^{(n)} - (-R^{(n+1)})\|^2$$

which is equivalent to (3.1).

Next we show that $\{C^{(n)}\}$ and $\{R^{(n)}\}$ are bounded. If not, let (i_0, j_0) be a minimal point in Ω (with respect to our partial ordering $\ll$) such that either $\{r_{i_0, j_0}^{(n)}\}$ or $\{c_{i_0, j_0}^{(n)}\}$ is unbounded. Say there exists a subsequence $\{n_i\}$ such that $r_{i_0, j_0}^{(n_i)} \longrightarrow -\infty$. (Since $\sum_{i=1}^{i_0} r_{i, j_0}^{(n)} \leq 0$ for all n (see Barlow and Brunk (1972)), $r_{i_0, j_0}^{(n_i)} \longrightarrow \infty$ would contradict the fact that (i_0, j_0) is minimal.) But this, together with $\widetilde{G}^{(n)} = G + R^{(n)} + C^{(n)}$ and the fact that $\widetilde{G}^{(n)}$ is bounded in norm (cf. (3.1)) implies that $c_{i_0, j_0}^{(n_i)} \longrightarrow \infty$. This, in turn, contradicts the fact that (i_0, j_0) is minimal since $\sum_{j=1}^{i_0} c_{i_0, j}^{(n)} \leq 0$ for all n.

Projections onto convex sets are distance reducing so that

$$\|C^{(i)} - C^{(i-1)}\|^2 = \|G + C^{(i)} - (G + C^{(i-1)})\|^2$$

(3.2)
$$\geq \|R^{(i+1)} - R^{(i)}\|^2 = \|G + R^{(i+1)} - (G + R^{(i)})\|^2$$

$$\geq \|C^{(i+1)} - C^{(i)}\|^2 \quad \text{for all } i.$$

We now show that

(3.3) $\quad \|R^{(i+1)} - R^{(i)}\|^2$ (and hence $\|C^{(i+1)} - C^{(i)}\|^2) \to 0$

$$\text{as } i \to \infty.$$

If (3.3) were not the case, there would exist $(i_0, j_0) \in \Omega$ and $\epsilon > 0$ such that

(3.4) $\quad |r_{i_0, j_0}^{(i+1)} - r_{i_0, j_0}^{(i)}| > \epsilon$ for infinitely many i.

However, since $\{R^{(n)}\}$ is bounded, there exists a finite M such that

(3.5) $\quad |r_{i_0, j_0}^{(i)} - r_{i_0, j_0}^{(j)}| < M$ for all i, j.

If we write

(3.6) $\quad \|R^{(i+1)} - R^{(i)}\|^2 - \|C^{(i+1)} - C^{(i)}\|^2$

$$= \|G + R^{(i)} + C^{(i)} - (G + R^{(i+1)} + C^{(i+1)}\|^2$$

$$+ 2(G + R^{(i)} + C^{(i)} - (G + R^{(i+1)} + C^{(i+1)}), C^{(i+1)} - C^{(i)}),$$

the left side of (3.6) converges to 0 since by (3.2) both terms converge to the same quantity. The last term of the right side is nonnegative by (2.1) and (2.2). Thus

(3.7) $\quad (R^{(i+1)} - R^{(i)}) + (C^{(i+1)} - C^{(i)}) \to 0$ as $i \to \infty$.

In similar fashion, beginning with

$$\|C^{(i+1)} - C^{(i)}\|^2 - \|R^{(i+2)} - R^{(i+1)}\|^2,$$

we can conclude

(3.8) $\quad (R^{(i+2)} - R^{(i+1)}) + (C^{(i+1)} - C^{(i)}) \longrightarrow 0 \quad \text{as} \quad i \longrightarrow \infty.$

Subtracting (3.7) from (3.8) yields

$$(R^{(i+2)} - R^{(i+1)}) - (R^{(i+1)} - R^{(i)}) \longrightarrow 0 \quad \text{as} \quad i \longrightarrow \infty.$$

Thus, for a sufficiently large N_0 and fixed n_0, we can keep

$$(r_{i_0,j_0}^{(N_0+1+i)} - r_{i_0,j_0}^{(N_0+i)}), \quad i = 1,2,\cdots,n_0$$

arbitrarily close to

$$(r_{i_0,j_0}^{(N_0+1)} - r_{i_0,j_0}^{(N_0)}).$$

This, however, contradicts (3.4) and (3.5) both being true.

Since $\{R^{(n)}\}$ and $\{C^{(n)}\}$ are bounded, there must exist convergent subsequences. Suppose $R^{(n_i)} \longrightarrow R$ and $C^{(n_i)} \longrightarrow C$. Then, in light of (3.3),

$$\widetilde{G}^{(n_i)} = G + R^{(n_i)} + C^{(n_i)}$$

and

$$\hat{G}^{(n_i+1)} = G + R^{(n_i+1)} + C^{(n_i)}$$

both converge to

$G^* = G+R+C$ (in anticipation of this being the desired solution).
Since $\hat{G}^{(n)}$ is an element of K_r and $\tilde{G}^{(n)}$ is an element of
K_c for all n, we know that $G^* \in K_r \cap K_c$ (these cones are
closed). Furthermore,

$$(G-G^*,G^*) = (G+R-G^*,G^*) - (R,G^*)$$

$$= \lim_{i \to \infty}(G+R^{(n_i)}-\tilde{G}^{(n_i)},\tilde{G}^{(n_i)}) + \lim_{i \to \infty}(G+C^{(n_i)}-\hat{G}^{(n_i+1)},\hat{G}^{(n_i+1)})$$

$$= 0 + 0.$$

Similarly, if $V \in K_r \cap K_c$,

$$(G-G^*,V) = (G+R-G^*,V) - (R,V)$$

$$= \lim_{i \to \infty}(G+R^{(n_i)}-\tilde{G}^{(n_i)},V) + \lim_{i \to \infty}(G+C^{(n_i)}-\hat{G}^{(n_i+1)},V) \leq 0 + 0.$$

Thus G^* is the desired solution by (2.1) and (2.2). Moreover,
since

$$-C \text{ minimizes } \|G + R - F\|^2, \quad F \in K_c^{*w}$$

and

$$-R \quad \text{minimizes} \quad \|G + C - F\|^2, \quad F \in K_r^{*W},$$

we may use the distance reducing property of projections to say

$$\|C^{(n)} - C\|^2 = \|G + C^{(n)} - (G+C)\|^2 \geq \|R^{(n+1)} - R\|^2$$

$$= \|G + R^{(n+1)} - (G+R)\|^2 \geq \|C^{(n+1)} - C\|^2 \quad \text{for all} \quad n.$$

Thus

$$R^{(n)} \to R \quad \text{and} \quad C^{(n)} \to C \quad \text{as} \quad n \to \infty$$

which implies that

$$\hat{G}^{(n)} = G + R^{(n)} + C^{(n-1)} \quad \text{and} \quad \tilde{G}^{(n)} = G + R^{(n)} + C^{(n)}$$

both converge to

$$G^* = G + R + C \quad \text{as} \quad n \to \infty.$$

4. OTHER POINTS. It is important to note that the solution $G^* = G + R + C$ does not uniquely determine R and C. In fact, if we begin with a column smoothing rather than row smoothing we will obtain different limiting values from R and C even though the same limiting G^* is obtained.

As one would expect, this procedure works equally well when

the order restrictions are modified to require nonincreasing
rows, or nonincreasing columns, or both. One has only to
change the one dimensional smoothing to operate in the appro-
priate direction. The procedure can also be adapted to higher
dimensions, although in this case the number of required
smoothings quickly becomes large.

We also wish to point out that G^* itself solves many more
minimization (maximization) problems than the least squares
problem stated above. For example, from Theorem 1.10 of Barlow
et al., if Φ is an appropriate convex function and φ is a
subgradient (basically a derivative) of Φ, then G^* solves
the problem

$$(4.1) \qquad \underset{F \in K_r \cap K_c}{\text{Maximize}} \quad \sum_{i=1}^{a} \sum_{j=1}^{b} \{\Phi(f_{ij}) + (g_{ij} - f_{ij})\varphi(f_{ij})\}w_{ij}.$$

Along somewhat similar lines, Theorem 3.1 of Barlow and
Brunk guarantees that the problem

$$(4.2) \qquad \underset{F \in K_r \cap K_c}{\text{Minimize}} \quad \sum_{i=1}^{a} \sum_{j=1}^{b} (\Phi(f_{ij}) - g_{ij} f_{ij})w_{ij}$$

is solved by $(\varphi^{-1}(g_{ij}^*))$ where once again Φ is an appropriate
convex function and φ is a subgradient of Φ.

Thus G^* solves a much wider range of problems than is
readily apparent. For example, suppose one has a multinomial
random vector X_{ij}, where the cell probabilities p_{ij} are
placed in a rectangular grid and one wishes to find the maximum

likelihood estimators for the p_{ij} subject to nondecreasing
(nonincreasing) rows and columns. This problem can be phrased
in terms of (4.1) from which it follows that the solution is
given by G^* where $G = (X_{ij}/n)$ and $w_{ij} \equiv 1$.

Similarly, if the X_{ij} are independent binomial (n_{ij}, p_{ij})
random variables, one can show that the maximum likelihood esti-
mators for the p_{ij} subject to nondecreasing (nonincreasing)
rows and columns is given by G^* where $G = (X_{ij}/n_{ij})$ and $w_{ij} = n_{ij}$.

Finally, in order to illustrate the algorithm on a larger
table, we considered the data presented in Table 4. The entries
are the first year grade point averages of 2397 students who
entered the University of Iowa in the Fall of 1978. The inde-
pendent variables are the composite scores on the ACT Assess-
ment and the student's high school percentile rank. The
expected first year grade point average is assumed to be a non-
decreasing function of both of these independent variables.
(The number in parentheses is the number of students in the
category.)

The least squares solution, correct to four significant
digits, was obtained after 500 iterations (250 row smoothings
and 250 column smoothings) at a cost of 9 seconds CPU time and
84 cents. These results are given in Table 5 with the level
sets indicated. Since the cost of our algorithm is essentially
linear in the number of points in the grid, even very large
arrays can be isotonized at a reasonable cost.

TABLE 4

First year GPA of students entering The University of Iowa as Freshmen in the Fall of 1978

High School Percentile Rank \ ACTC	1-12	13-15	16-18	19-21	22-24	25-27	28-30	31-33	34-36
91 ≤ HSR ≤ 99	1.57(4)	2.11(5)	2.73(18)	2.96(39)	2.97(126)	3.13(219)	3.41(232)	3.45(47)	3.51(4)
81 ≤ HSR ≤ 90	1.80(6)	1.94(15)	2.52(30)	2.68(65)	2.69(117)	2.82(143)	2.75(70)	2.74(8)	(0)
71 ≤ HSR ≤ 80	1.88(10)	2.32(13)	2.32(51)	2.53(83)	2.58(115)	2.55(107)	2.72(24)	2.76(4)	(0)
61 ≤ HSR ≤ 70	2.11(6)	2.23(32)	2.29(59)	2.29(84)	2.50(75)	2.42(44)	2.41(19)	(0)	(0)
51 ≤ HSR ≤ 60	1.60(11)	2.06(16)	2.12(49)	2.11(63)	2.31(57)	2.10(40)	1.58(4)	2.13(1)	(0)
41 ≤ HSR ≤ 50	1.75(6)	1.98(12)	2.05(31)	2.16(42)	2.35(34)	2.48(21)	1.36(4)	(0)	(0)
31 ≤ HSR ≤ 40	1.92(7)	1.84(6)	2.15(5)	1.95(27)	2.02(13)	2.10(13)	1.49(2)	(0)	(0)
21 ≤ HSR ≤ 30	1.62(1)	2.26(2)	1.91(5)	1.86(14)	1.88(11)	3.78(1)	1.40(2)	(0)	(0)
HSR ≤ 20	1.38(1)	1.57(2)	2.49(5)	2.01(7)	2.07(7)	(0)	.75(1)	(0)	(0)

TABLE 5

Least squares doubly nondecreasing regression function

1.87	2.17	2.73	2.96	2.97	3.13	3.41	3.45	3.51
1.87	2.17	2.52	2.68	2.69	2.79	2.79	2.79	2.79
1.87	2.17	2.32	2.53	2.57	2.57	2.72	2.76	2.76
1.87	2.17	2.29	2.29	2.46	2.46	2.46	2.46	2.46
1.73	2.06	2.12	2.13	2.25	2.25	2.25	2.25	2.25
1.73	1.98	2.05	2.13	2.25	2.25	2.25	2.25	2.25
1.73	1.94	1.98	1.98	2.02	2.05	2.05	2.05	2.05
1.62	1.94	1.96	1.96	1.96	2.05	2.05	2.05	2.05
1.38	1.57	1.96	1.96	1.96	1.96	1.96	1.96	1.96

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